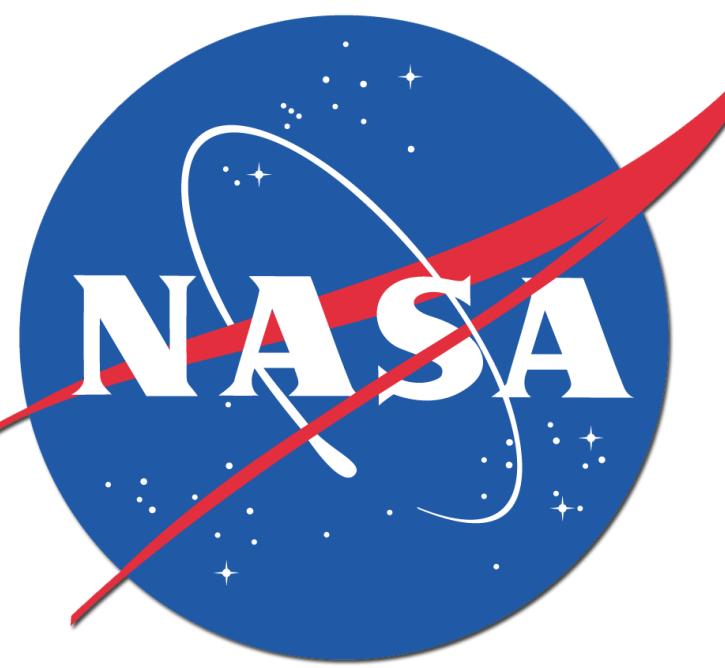




# Chemistry Simulations using the MERRA-2 Reanalysis with the GMI CTM and Replay in Support of the Atmospheric Composition Community



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## Summary

Simulations using reanalysis meteorological fields have long been used to understand the causes of atmospheric composition change in the recent past. Using the new MERRA-2 reanalysis, we are conducting chemistry simulations to create products covering 1980-2016 for the atmospheric composition community.

These simulations use the Global Modeling Initiative (GMI) chemical mechanism in two different models: the GMI Chemical Transport Model (CTM) and the GEOS-5 model in Replay mode. Replay mode means an integration of the GEOS-5 general circulation model that is incrementally adjusted each time step toward the MERRA-2 reanalysis. The GMI CTM is a  $1^\circ \times 1.25^\circ$  simulation and the MERRA-2 GMI Replay simulation uses the native MERRA-2 grid of approximately  $1/2^\circ$  horizontal resolution on the cubed sphere.

A specialized set of transport diagnostics is included in both runs to better understand trace gas transport and its variability in the recent past.

## Driven by MERRA-2 Meteorology

Both the CTM and Replay are driven by meteorology from the Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) meteorology. MERRA-2 is a global reanalysis of 1980 to the present using modern hyperspectral radiance and microwave observations, along with GPS-Radio Occultation datasets. The presence of an internally generated QBO in the general circulation model improves the representation of transport in the tropics and subtropics compared to previous simulations.

## Specialized Diagnostics and Output Collections

In addition to chemical constituents, the GMI CTM and Replay simulations include a suite of tracers sensitive to tropospheric and stratospheric transport processes on a range of time and spatial scales. Some of the tracers are:

**CH<sub>3</sub>I** - Marine convection tracer. Emitted over oceans with a 5-day e-fold.

**Rn/Pb** - Land-based convection tracer (Rn) with a 5.5 day e-fold, decaying to Pb, which is lost through washout.

**e90** - Tropospheric transport tracer emitted at the surface with a 90-day e-fold. It is used to identify the tropopause (Prather et al., JGR, 2011).

**Mean Age** - a pulsed and a clock tracer - For transport pathways and timescales.

**SF<sub>6</sub>** - Emitted at the surface with a large interhemispheric gradient. No losses.

**Strat O<sub>3</sub>** - This tracer is equal to model-calculated O<sub>3</sub> at the tropopause. In the troposphere, it has no source but undergoes loss based on interannually-varying monthly mean loss rates archived from a simulation with interactive chemistry.

Simulations have specialized collections that include high frequency 3-hrly (replay) and daily (CTM) output for a number of important constituents, daily satellite overpass output, and station data (hourly for some CTM species). Monthly mean output is available for all constituents.

Contact Luke Oman and Susan Strahan for more information.

## Availability

These simulations are done in support of the Atmospheric Composition Community and we appreciate feedback on their use.

GMI CTM output will be available in early 2017 via anonymous ftp from dirac.gsfc.nasa.gov. The directory is /pub/gmidata2/users/mrdamon/Hindcast-Family/HindcastMR2.

Contact Susan Strahan (susan.strahan@nasa.gov) for additional information and support.

The Replay simulation will be available in early 2017 using similar downloading mechanisms as MERRA-2 Reanalysis (i.e. OPeNDAP and web-based interfaces)

For more information see: <http://acd-ext.gsfc.nasa.gov/Projects/GEOSCCM/MERRA2GMI/> or contact Luke Oman (luke.d.oman@nasa.gov)

## CTM Overview

A simulation using the GMI chemistry transport model (CTM) driven by MERRA-2 meteorological fields is currently underway and will be completed in early 2017. MERRA-2 met fields driving the CTM are 3-hr averages (e.g., u,v,T) with no interpolation between the 3-hr updates. This differs from Replay (see below). This simulation used the native MERRA-2 vertical coordinate (72 levels) with horizontal resolution  $1^\circ \times 1.25^\circ$ . The updated GMI chemical mechanism (JPL 2015) contains 124 species, 322 kinetic and 81 photolytic reactions. MERRA-2 aerosols are used in the troposphere and IGAC sulfate aerosols are used in the stratosphere.

Initial GMI-MERRA-2 results will soon be available. To the right (blue) we present examples of analyses done with the GMI CTM integrated with MERRA fields.

## Replay Overview

We are integrating a simulation using the GMI chemical mechanism and the GEOS-5 model in Replay mode at  $1/2^\circ$  horizontal resolution on the cubed sphere; outputs have the same  $0.625^\circ \times 0.5^\circ$  grid as the MERRA-2 Reanalysis. Replay requires running two forecasts with the GEOS-5 model.

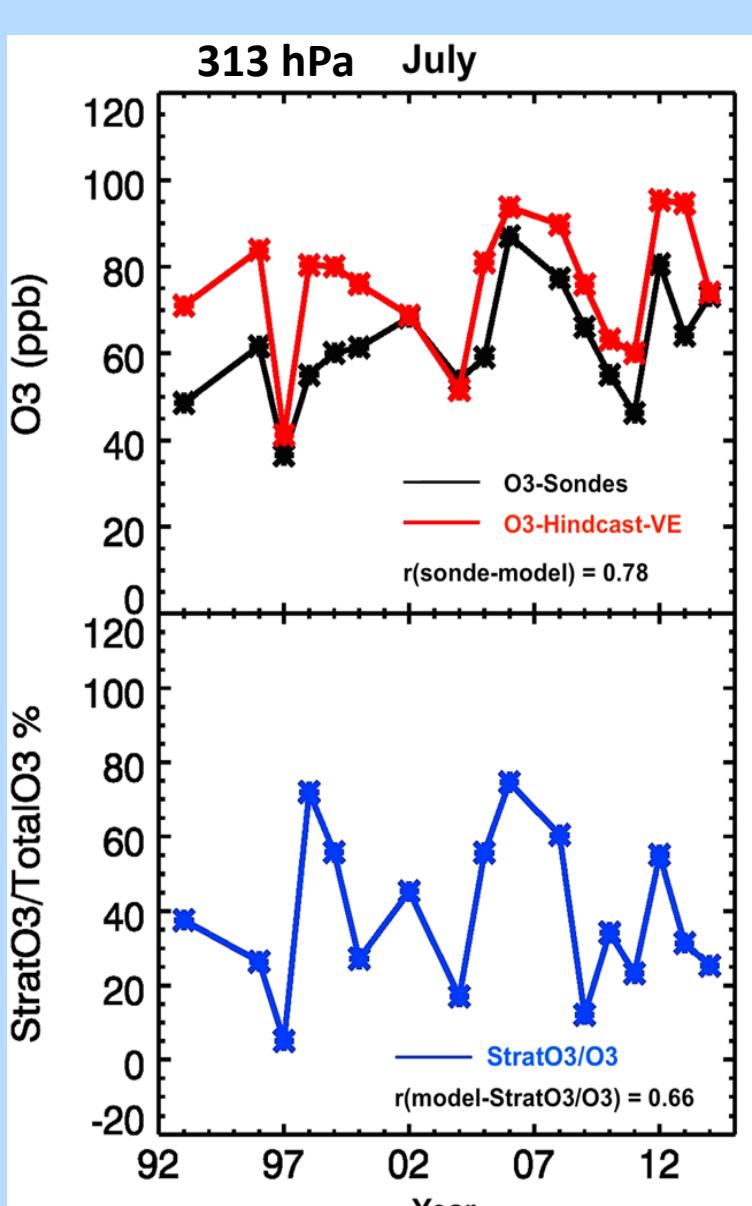
The first forecast calculates the background model predicted state (bkg), which then is compared to the assimilated state (asm) from time averaged MERRA-2 fields (u,v,t,pressure + others which are optional).

The difference between bkg and asm divided by the number seconds elapsed produces the Incremental Analysis Unit (IAU). This is applied to the "replayed" variables at each time step (IAU \* time step) as the model is run forward again. The user chooses the frequency of "replaying" but for this simulation we use 3-hour intervals.

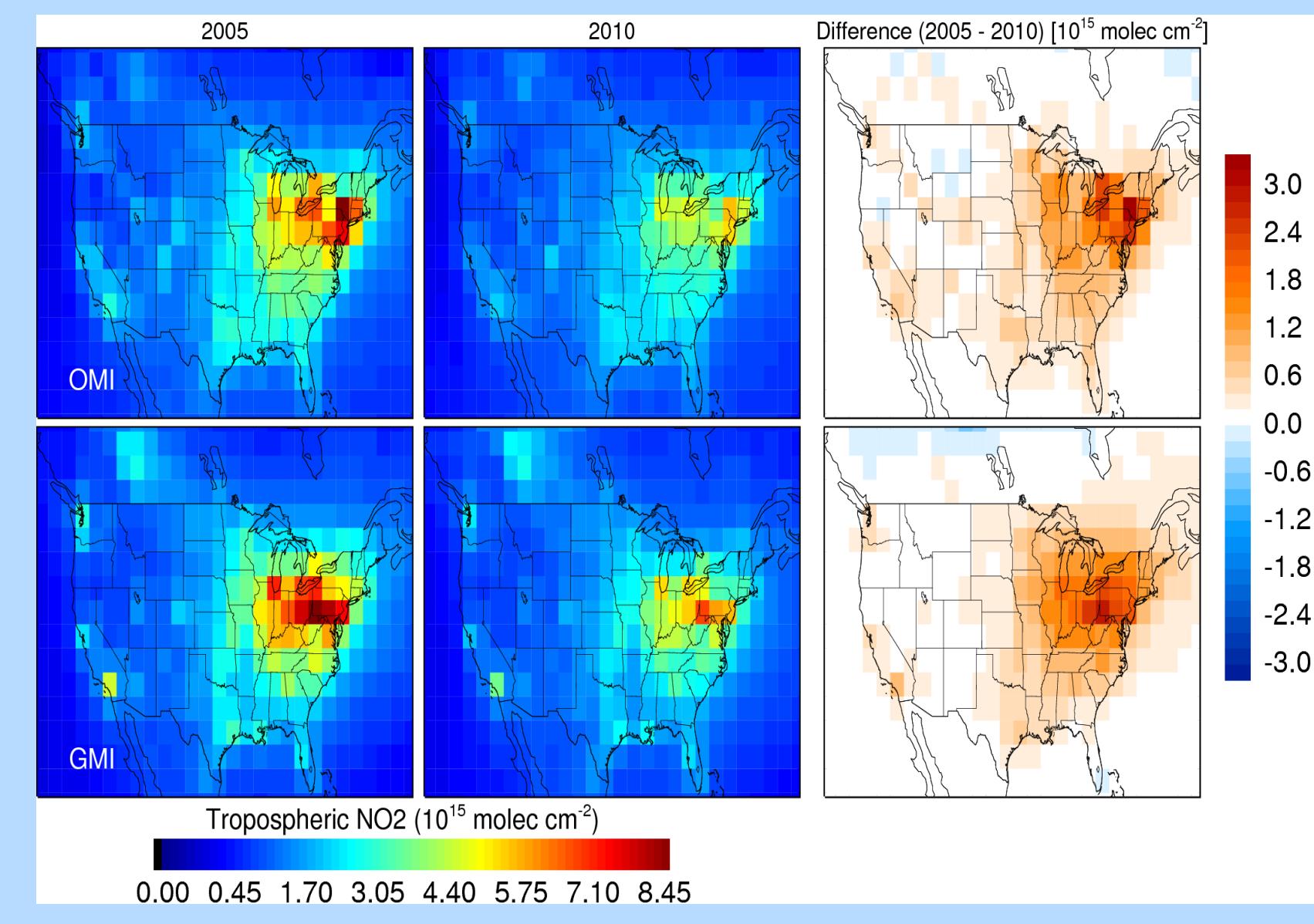
## GMI-MERRA CTM Examples

**GMI Strat Ozone tracer shows the contribution of stratospheric O<sub>3</sub> to tropospheric O<sub>3</sub> trends**

(Right) This figure shows good agreement between the time series of observed upper tropospheric O<sub>3</sub> (313 hPa) from Reunion Island (21°S) sondes (black) and GMI-MERRA simulated ozone (red) [top]. The bottom panel shows the StratO<sub>3</sub> tracer/O<sub>3</sub> ratio (blue), indicating the fraction of upper tropospheric ozone that originated in the stratosphere. The model results are sampled on the dates of sonde measurements. From J. Liu et al., JGR, 2016.

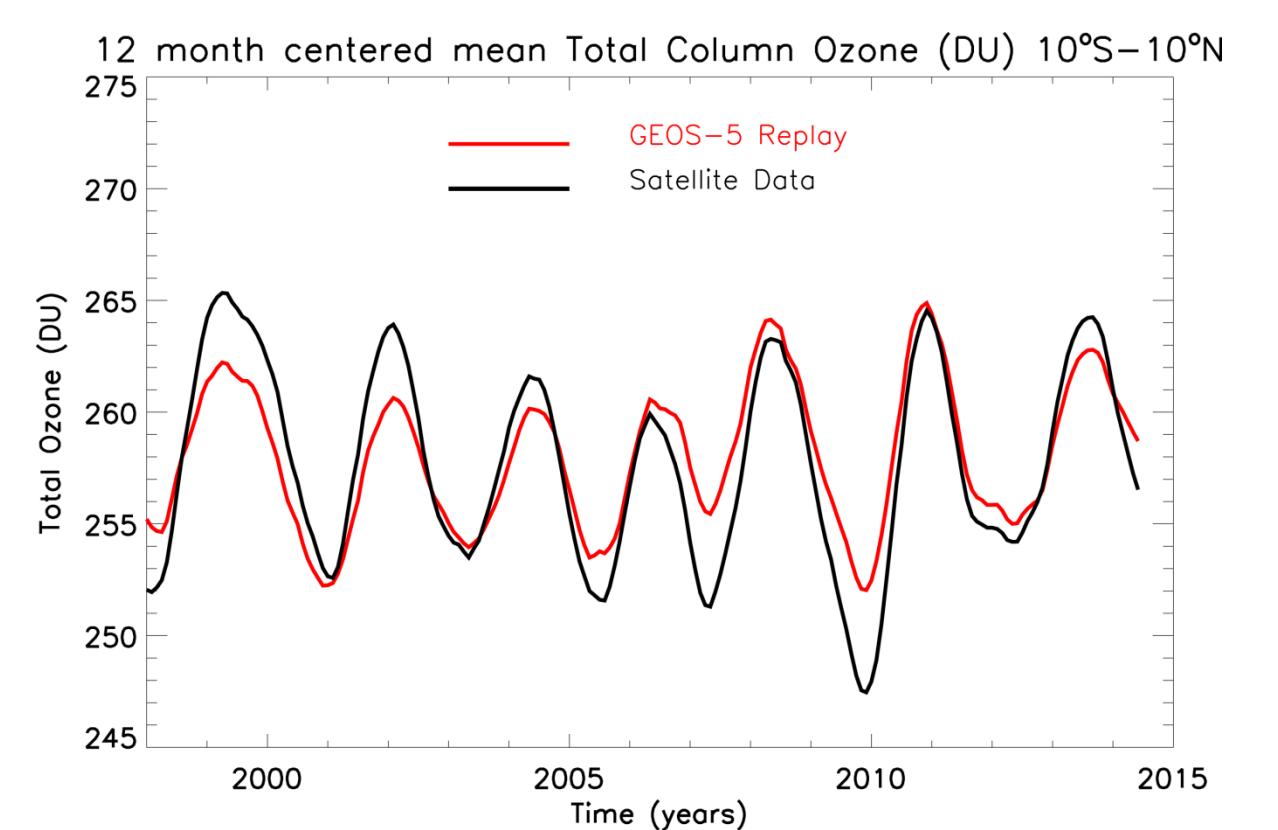
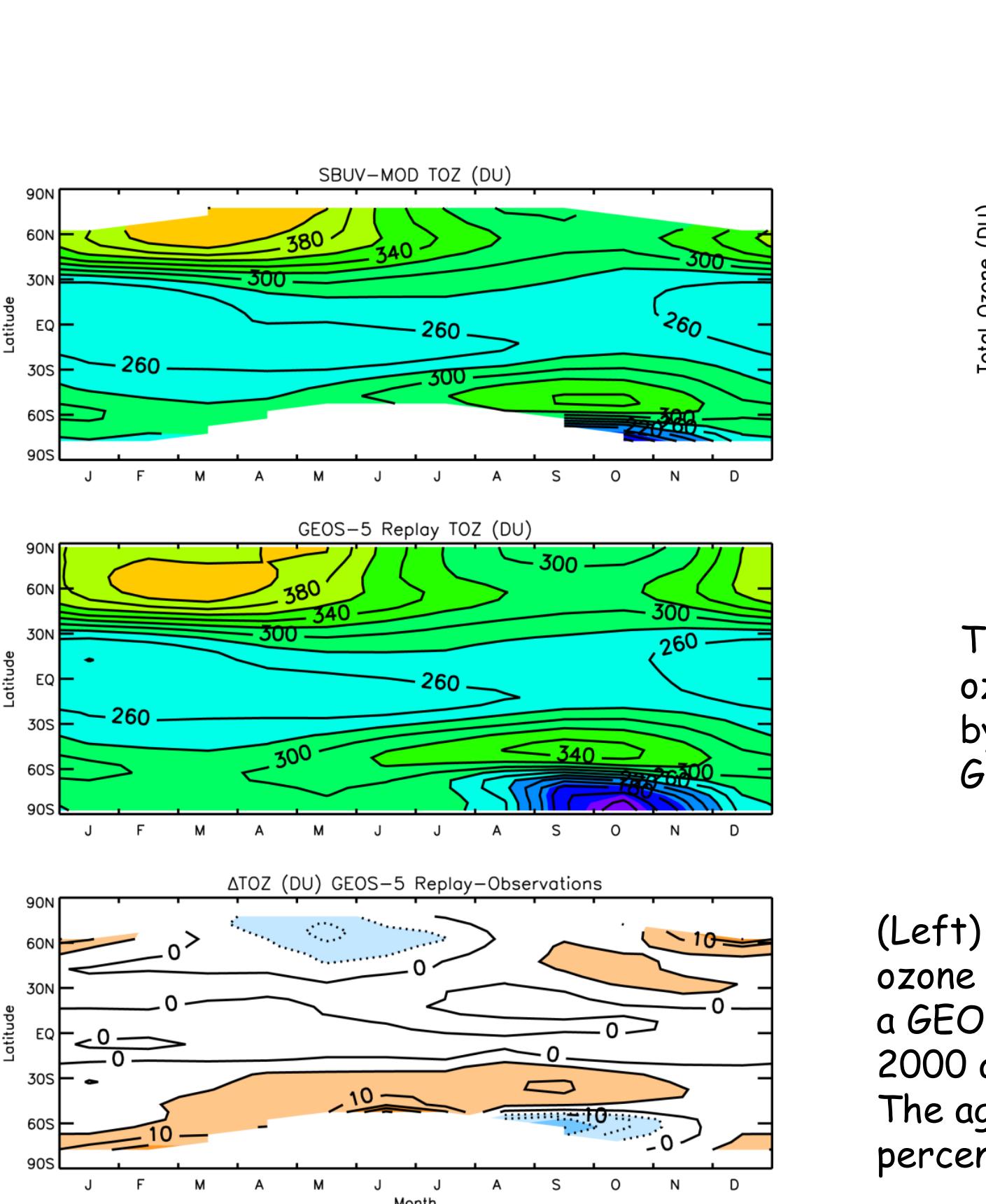


**GMI-MERRA Hindcast simulates tropospheric NO<sub>2</sub> columns (bottom) that compare well with OMI (top).**



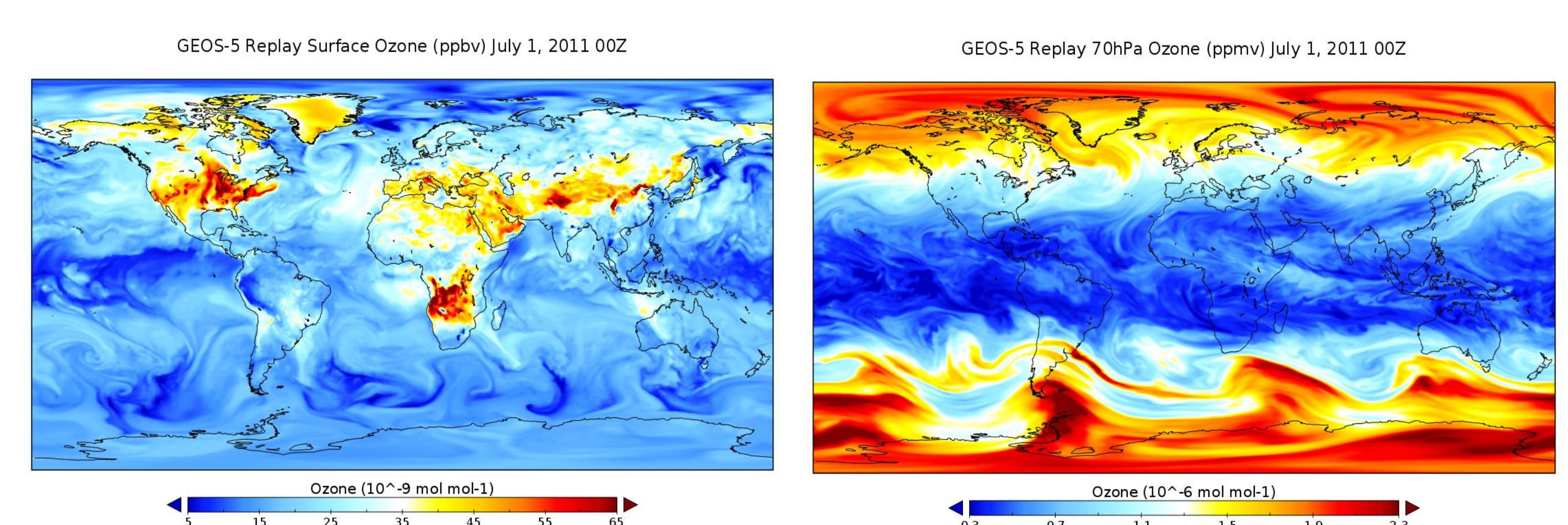
The simulation captures the observed trend in NO<sub>2</sub> reduction in the Ohio Valley from 2005-2010 (right column). Simulated NO<sub>2</sub> is sampled at the OMI overpass time. From Strode et al., JGR, 2015.

## Replay Examples



The figure above shows the tropical total column ozone interannual variability, which is dominated by the QBO and is largely reproduced in a GEOS-5 Replay scout simulation.

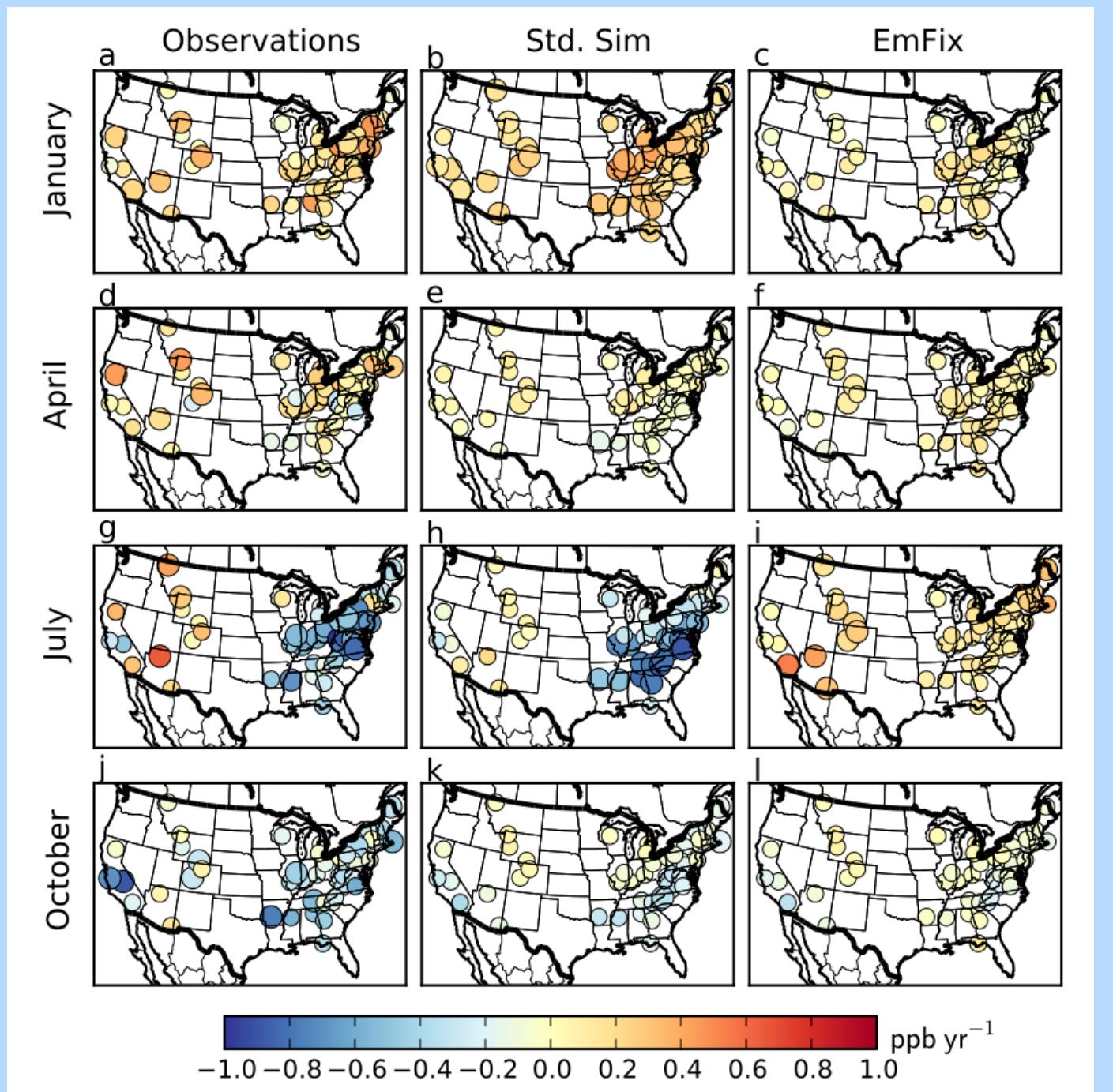
(Left) These figures show an example of total column ozone from the SBUV-MOD data set (top) compared to a GEOS-5 Replay scout simulation (middle) for 1998-2000 and the difference between the two (bottom). The agreement is very good and generally within a few percent of observations.



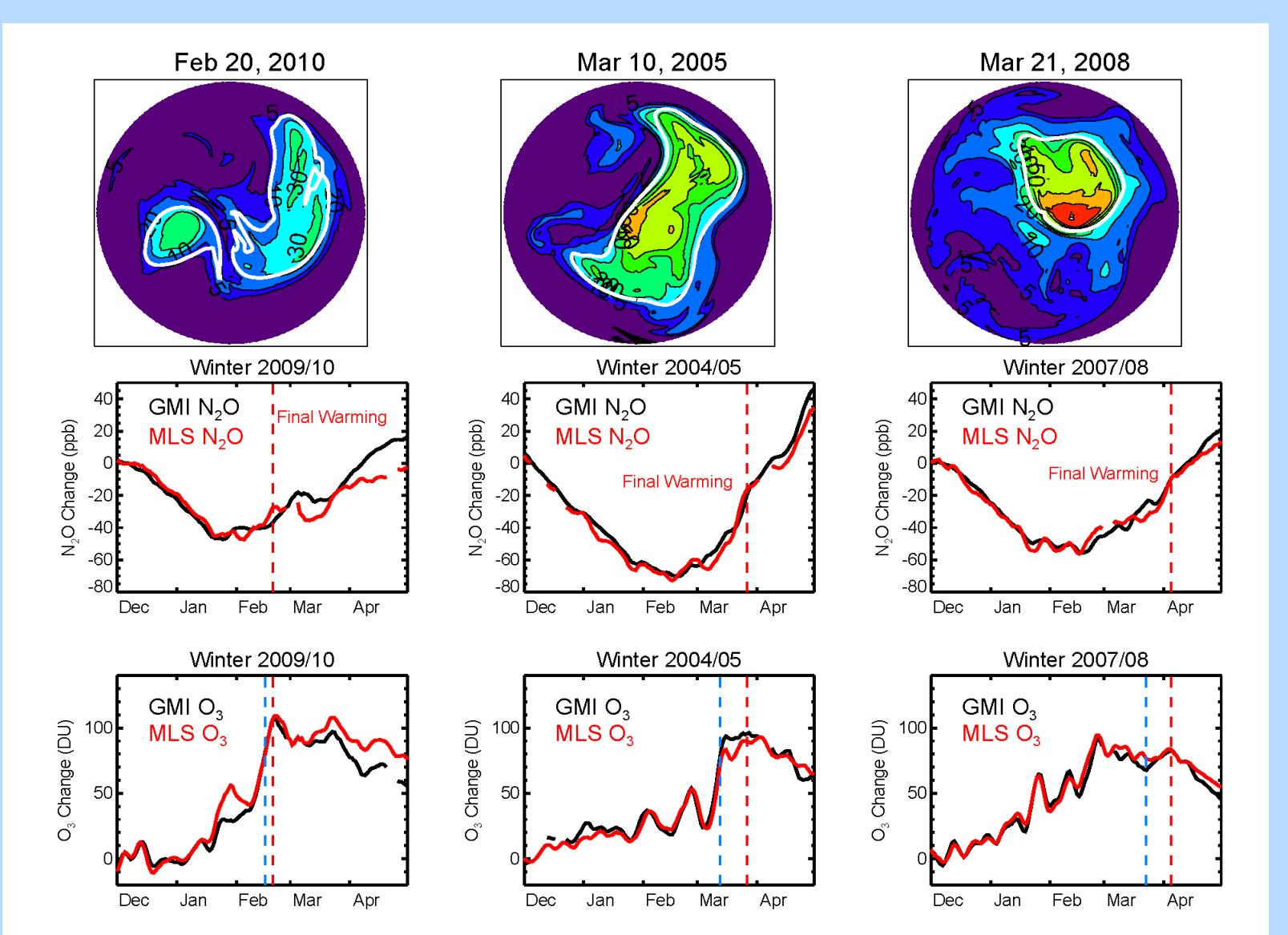
The figures above show examples of surface (left) and 70 hPa (right) ozone from a test GEOS-5 Replay simulation for July 1<sup>st</sup>, 2011, showing resolved structures in the boundary layer and lower stratosphere.

**(Right) The observed negative ozone trends in the eastern U.S. in summer are present in the GMI Hindcast (Std Sim) but are absent from a fixed emissions (EmFix) simulation, confirming the role of emission reductions in reducing summertime ozone.**

Trends in monthly median daytime ozone for 1991-2010 in surface observations (left column), standard simulation (middle column), and EmFix simulation (right column), and the difference between them (bottom row). Larger circles indicate that the trend is statistically significant. From Strode et al., JGR, 2015.



**Excellent Representation of polar stratospheric chemistry and transport allows quantitative separation of polar ozone depletion from ozone transport variations**



These figures from a GMI-MERRA simulation [Strahan et al., JGR, 2016] show polar O<sub>3</sub> depletion (DU) in 3 Arctic winters during the Aura period, along with comparisons to MLS N<sub>2</sub>O and O<sub>3</sub>.

The depletion (top row) is the difference between 2 GMI simulations, one with and one without heterogeneous halogen reactions.

The excellent agreement between MLS and GMI N<sub>2</sub>O and O<sub>3</sub> during 3 Arctic winters demonstrates the credibility of vortex descent and isolation (middle row) and the O<sub>3</sub> resupply and depletion (bottom row). Line plots show the change since December 1 in 450 K N<sub>2</sub>O and column O<sub>3</sub> averaged over the Arctic vortex. The dashed blue line indicates when temperatures became too high for halogen activation on cloud particles.